Gobas Food Web Model Default Values for Model Parameters

The following text summarizes the limited number of site-specific data inputs required by the Gobas food web model (FWM), as well as the remaining model parameters which have assumed default values set by Gobas and co-workers. For this purpose, I've used the publically available version of the Gobas FWM, (called AQUAWEB v1.2 at the Simon Fraser University website where the model can be downloaded, http://www.rem.sfu.ca/toxicology/models/aquaweb/), the version that became available in 2007. It's the version that should have been used as the basis for the visual basic code from the July 2009 FWM memorandum. The 2007 iteration of the FWM has two minor code changes compared to the originally published Arnot and Gobas (2004) model:

1. Different way of converting non-lipid organic matter to non-lipid organic carbon content in the gut
2. Change in model assumption for density of lipids. The updated 2007 FWM assumes a default lipid density of 0.9 kg/L. This corrects a minor error in the Arnot and Gobas 2004 model code, which assumed lipid and water both had a default density of 1.0 L/kg.

The absolute minimum number of site- and chemical-specific parameters that must be entered into the Gobas FWM for it to function are the following:

Chemical properties:

- octanol-water partition coefficient (K_{OW})
- Henry's Law constant (although this cancels itself out during calculation, thus is not absolutely essential)

Site-specific environmental properties:

- mean water temperature
- concentration of particulate organic carbon in the water
- concentration of dissolved organic carbon in the water
- concentration of suspended solids in the water
- organic carbon content of the sediment
- chemical concentration in the water
- chemical concentration in the sediment

Site-specific biological properties for each species modeled (the default Gobas model can make predictions of tissue contaminant concentrations for up to 14 fish species, 5 invertebrate species, zooplankton and phytoplankton):

- organism wet weight
- organism lipid content
- organism feeding preferences

The number of user entered parameters therefore varies depending on how many chemicals and species are modeled in each model run.

As there are no Portland Harbor specific measurements on the biological properties of phytoplankton and zooplankton, model default values for biological properties for trophic levels 1 (phytoplankton) and 2 (zooplankton) should be Gobas model default values. Several other parameters, such as the mean dissolved oxygen content of site water, are also site specific if the information is available. If not available, the model calculates them from other input data. For example, if measured dissolved oxygen data are unavailable, the dissolved oxygen concentration is calculated from user entered water temperature data and a model default value for the oxygen saturation percentage.

Any or all other model parameters can be modified using site-specific information if it is available. Much of the Portland site-specific information comes from the species whose tissue contaminant concentrations are modeled. However, a number of the model parameters, such as the lipid density of 0.9 L/kg discussed earlier, are normally retained at the Gobas FWM default values.

EPA has previously recommended in its comments to the LWG that unless site-specific information is available for a model parameter, the Gobas default value for each model parameter be retained. Those model default values for the 21 internal model parameters EPA expressed concern about in our comments on the FWM as being changed from model defaults without an explicit site-specific reason to do so are in the spreadsheet that is a companion to this memorandum.

Of the 21 internal model parameters we expressed concern about during the 2007 – 2009 time period, only two appear not to have been reset to Gobas model default values. They are:

- Dietary absorption efficiency of lipid by zooplankton: Gobas default = 0.75, current LWG value = 0.72.
- Dietary absorption efficiency of non-lipid organic matter (NLOM) by zooplankton: Gobas default = 0.75, current LWG value = 0.72.

The remaining model parameters appear to be either chemical-specific values such as the log K_{OW} for a chemical, species-specific values such as body weights or the dietary fractions of different prey species in the diet of a modeled species, or site-specific environmental values such as mean water temperature or sediment PCB concentration, or parameters whose values the model calculates from the values entered for species- or site-specific values. Comparison of these types of model parameter values to the Gobas default values has little or no utility, since the FWM would not be site-specific without these site-specific input values.

Most if not all of the chemical-, species- and site-specific parameter values have been discussed with the LWG at length during development of the FWM. Among the model parameters having the greatest impact on model predictions of tissue contaminant concentrations, they are either measured at the site (e.g. PCB in sediment concentrations, lipid content in smallmouth bass, etc.) or have been agreed to between LWG and EPA (e.g. log K_{OW} values, dietary fractions of prey

species in the diet of a modeled species, etc.). I'm comfortable with the dietary preferences of the modeled species in LWG's modeling efforts. After all, it is a food web that is being modeled, and it wouldn't be very useful if we had piscivorous species such as northern pikeminnow or smallmouth bass feeding largely on zooplankton. As I've stated many times, I believe the largest single source of uncertainty in the FWM predictions results from the relative lack of empirical fish and invertebrate tissue contaminant data relative to the amount of empirical sediment contaminant data available for the site.